Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Automated generation of quantum-accurate classical interatomic potentials for metals and semiconductors[1] AIDAN THOMPSON, STEPHEN FOILES, PETER SCHULTZ, LAURA SWILER, CHRISTIAN TROTT, GARRITT TUCKER, Sandia National Laboratories — Molecular dynamics (MD) is a powerful condensed matter simulation tool for bridging between macroscopic continuum models and quantum models (QM) treating a few hundred atoms, but is limited by the accuracy of available interatomic potentials. Sound physical and chemical understanding of these interactions have resulted in a variety of concise potentials for certain systems, but it is difficult to extend them to new materials and properties. The growing availability of large QM data sets has made it possible to use more automated machine-learning approaches. Bartók *et al.* demonstrated that the bispectrum of the local neighbor density provides good regression surrogates for QM models. We adopt a similar bispectrum representation within a linear regression scheme. We have produced potentials for silicon and tantalum, and we are currently extending the method to III-V compounds. Results will be presented demonstrating the accuracy of these potentials relative to the training data, as well as their ability to accurately predict material properties not explicitly included in the training data.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Dept. of Energy Nat. Nuclear Security Admin. under Contract DE-AC04-94AL85000.

Aidan Thompson
Sandia National Laboratories

Date submitted: 09 Nov 2012 Electronic form version 1.4